EQUiPS Proposers' Day

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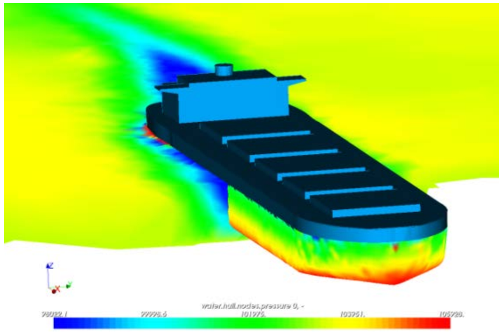
Important Disclaimer

- In the event of a disagreement between the contents of the anticipated BAA and the information in this briefing, **please follow the BAA**. No exceptions.

Program Motivation and Overview

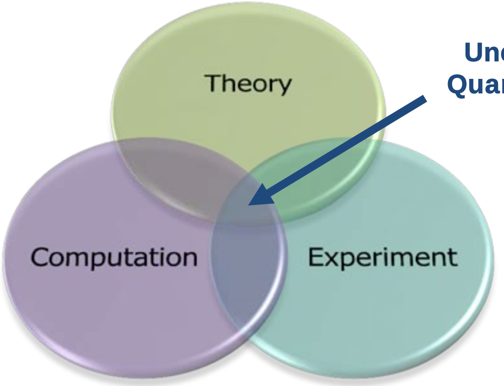
The Need for Uncertainty Quantification (UQ)

- Computation has become the "third pillar" of science after theory and experiment.
- It has proven effective in solving large scale, coupled, physics equations where there is no hope for an analytic solution, or experiments are either too expensive or impossible to perform.



Computational Fluid Dynamics (CFD) simulation for ship navigation simulation.

But computational modeling is not yet predictive.



To perform accurate predictions and risk-informed decision making, we must perform Verification and Validation (V&V) on computational results that

- incorporate natural uncertainties,
- combine computation with theory and observational data for increased predictive power.

Computational science must be augmented with the mathematics of Uncertainty Quantification.

Current Approach: The Forward Model

Physical System Described by Partial Differential Equations

$$\begin{cases} -\operatorname{div}(a(x,\mathbf{y})\nabla u(x,\mathbf{y})) = f(x), & x \in D, \\ u(x,\mathbf{y}) = 0, & x \in \partial D \end{cases} \quad \forall \mathbf{y} \in \Gamma \subset \mathbb{R}^N$$

uncertain coefficients

uncertain boundary conditions

unknown function

forcing function

random variable parameterizing uncertainty

Estimate the average (variance, etc.) of a Quantity of Interest (QoI) g(u), say:

$$g(u) = \int_{\mathcal{D}} \kappa(\mathbf{x}) u(\mathbf{x}) d\mathbf{x}$$

Option 1: Monte Carlo

- Sample y M times as necessary for desired confidence (say, 95%) and tolerance:

$$M_{95\%} \sim \frac{2\hat{\sigma}^2}{Tol^2}$$

- Solve PDE for u M times.
- Compute g(u) M times. Take average, Ê[g].
- Central Limit Theorem “says”:

$$E[g] = \hat{E}[g] \pm Tol$$

Option 2: Polynomial Expansions

- Express the solution as an infinite sum of deterministic and stochastic contributions

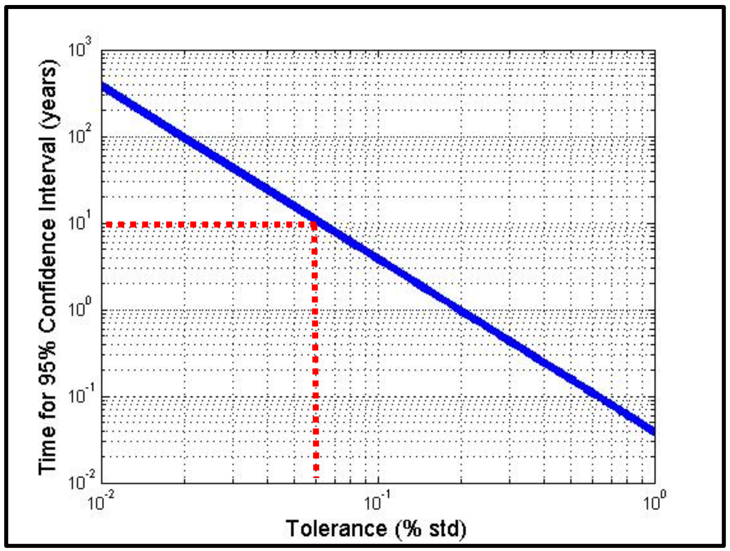
$$u(x,\mathbf{y}) = \sum_{i=0}^{\infty} u_i(x)\psi_i(\mathbf{y})$$

- Truncate the series at P terms to get P+1 coupled and deterministic equations for P unknowns.
- From these, extract the moments of u, and compute QOIs.

Shortcomings of Current SOA

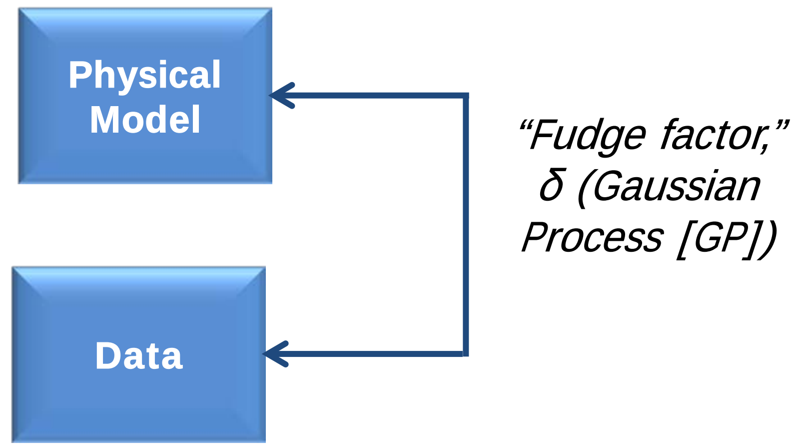
Scalability

- For a high dimensional simulation (~1 week), statistically significant (Tolerance <4% std.) results take years.



Model Form Uncertainty (MFU)

- How are the input distributions generated in the first place? We need inverse methods.
- ***All models are approximate.***
- How can we possibly quantify model uncertainty and inadequacy?

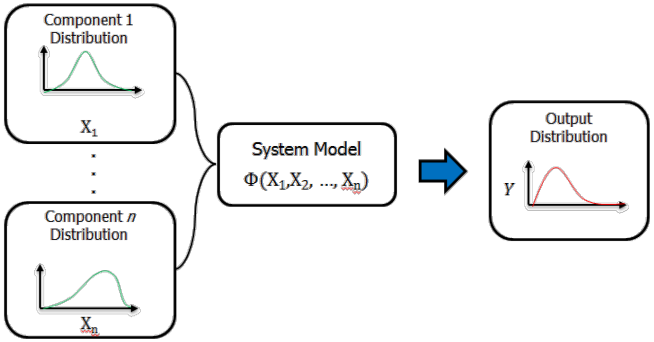


Lack of Design and Decision Under Uncertainty Methods

- There is no computationally effective and mathematically rigorous framework for design under uncertainty for large complex systems. Instead, costly and repetitive testing is used.

EQUiPS Vision

EQUiPS will create the basic **mathematics** needed to efficiently quantify, propagate and manage multiple sources of (parametric and model) uncertainty to make accurate predictions about (and design) complex DoD systems.



EQUiPS will develop:

- **TA#1**: New methods for forward and inverse modeling to scale to very-high-dimensional (10^4-10^6) multiscale/multiphysics systems.
- **TA#2**: A quantitative understanding of uncertainties in the physical models themselves.
- **TA#3**: A completely new paradigm for stochastic design and decision making for complex systems.

Abstract and Proposal Guidance

EQUiPS Thrust Areas

EQUiPS is a 3-year program (executed in two, 18-month phases) that will focus on creating core mathematical methodologies for the effective deployment of UQ in large, multi-physics/scale DoD systems.

EQUiPS consists of three Thrust Areas (TAs) which will rectify current shortcomings by leveraging:

TA#1: Scalable Algorithms

- Recent advances in stochastic PDEs with multiscale structure.
- New results that combine many samples from low fidelity models with few computationally intensive samples from high fidelity ones.
- Novel methods for characterizing the error introduced by surrogate models.
- Recent methods from sparse optimization that suggest methods to determine the optimal sampling or stochastic model approach to a given UQ problem.

TA#2: Model Form Uncertainty

- Approaches that use physical considerations (conservation laws, symmetries) to massively dimensionally reduce the possible form of the model mismatch.
- New Bayesian inversion methods for simultaneous model calibration and model mismatch fitting.
- Advances in approximate and fast model fitting techniques such as belief propagation and simulated annealing to allow fast inference for more nuanced models than the Gaussian Process.

EQUiPS Thrust Areas

EQUiPS consists of three Thrust Areas (TAs) that will rectify current shortcomings by leveraging:

TA#3: Design and Decision-Making Under Uncertainty

- Gains of TA#1 and TA#2 to massively increase the speed of the “inner loop” of the design process.
- Importance sampling, extreme value theory and concentration of measure theory, to develop new methods for ***rare events*** to implement risk-based design.
- New approaches to stochastic optimization that allow optimization of entire probability distribution functions, instead of just low-order moments.
- New multi-information-source stochastic optimization techniques.

All teams must address all TAs in their abstracts/proposals.

Phases and Teaming

- In Phase I, teams should focus on basic theoretical developments; the goal of this phase is to create a new mathematical formalism for DoD-scale UQ along with new fundamental insights into model-form uncertainty and design.
- During Phase II, performers will continue to develop mathematical and theoretical gains, while simultaneously focusing on design, and, in particular, engaging with the DoD design challenges in their chosen application areas (more below).

Teams are expected to be interdisciplinary and integrated, including sufficient expertise to tackle all program aspects.

Application and Design Domain

- Each team must select and specify an "application and design domain."
- These must involve multi-physics/scale physical phenomena.
- Example application areas might include (but are not limited to):
  - ❑ Aerospace structures
  - ❑ Engines
  - ❑ Marine vehicles
  - ❑ Radar and electromagnetic scattering
  - ❑ Material discovery
  - ❑ Biological systems

Teams are strongly encouraged to choose only one specific application area in which they will concentrate.

Application Test-Cases

- Teams will be required to demonstrate their algorithms on a complex UQ problem test-case (which should be described in detail in the abstract/proposal) from their chosen Application and Design domain.

- In Phase I, a forward UQ analysis of the test-case should be conducted.

- In Phase II, more complexity should be added to the test-case (for example, generalizing a 2D system to 3D). In addition to the forward UQ analysis, teams should implement:
  - ❑ Inverse UQ analysis
  - ❑ Model-form uncertainty techniques
  - ❑ Design studies

DARPA Application Team

- In addition to the work performed in TAs 1-3, and the application test-cases, DARPA will work with an "Application Team" to develop a set of DoD design challenges based on the performers' proposed application and design domains that capture the complexity and subtlety of real UQ and design problems.
- In Phase I, teams should make themselves available (for meetings, site visits, telecons, etc.) with the DARPA Application Team, with whom they will work closely to help devise relevant DoD design challenges.
- In Phase II, the challenges will be released to each team.

Note, DARPA is not accepting proposals for the Application Team under this BAA.

EQUiPS Broad Technical Milestones (all teams must address)

Thrust Area	Phase I Milestones	Phase II Milestones
TA1 Scalable Algorithms	• new dimensional reduction methods with theoretical error bounds; • scalable Bayesian inference algorithms (for inverse problems) with orders of magnitude speed-up incorporating the structure/physics of the problem; • UQ algorithms on emerging high-performance computing platforms; and • forward UQ on a multi-scale system test-case with coupled physics in chosen application areas.	• optimal (with respect to both efficiency and accuracy) UQ methodologies under computing resource constraints; • forward and inverse UQ techniques in the context of a multi-scale system with coupled physics for chosen test-case; and • algorithms in DoD design challenges provided by the DARPA Application Team.
TA2 Model-Form Uncertainty	• proofs of theorems regarding methods for model-form uncertainty that go beyond the Gaussian Process; • multi-fidelity techniques for model error estimation; • physics-based methods for model-form uncertainty; and • new techniques for detection of rare events.	• model-form uncertainty techniques and multi-fidelity approaches for chosen test-case; and • algorithms in DoD design challenges provided by the DARPA Application Team.
TA3 Design and Decision Making under Uncertainty	• a new theoretical framework for stochastic optimization/risk averse optimization; • multi-fidelity approach in the context of stochastic optimization; • proofs and theoretical treatment of rare event detection algorithms within risk-based optimization framework; and • design techniques for a nominal design problem related to the test-case.	• design techniques for chosen test-case; and • algorithms in DoD design challenges provided by the DARPA Application Team.

EQUiPS Detailed Technical Milestones (performer specific)

The particular milestones and schedules of each individual team will be proposer specific. All full proposals must contain:

- Thorough documentation and references supporting existing state of the art metrics for their chosen UQ and design methods.
- A detailed technical plan and schedule for achieving orders of magnitude beyond this SOA.
- A quantitative table such as the one below (example only; this will be performer specific):

Thrust Area	Sub-area	Quantitative Milestone	Month Delivered
I	New sampling strategies	10x speedup over MC	6
I	Dimensional reduction/surrogate modeling	System with 10K parameters with <5% loss in accuracy	6
I	Scalable inverse techniques	Systems with 10k parameters	9
I	New results on optimal UQ methods	N/A	12
I	UQ demonstration	A system with different length/time scales	18
I	New sampling strategies	1000x speedup over MC	18
I	Dimensional reduction	System with 100K parameters with <5% loss in accuracy	23
I	Prove optimality for UQ framework	N/A	30
I	UQ demonstration	Multi-scale system with >1M parameters	36
II	Methods for model-form uncertainty	Outperform GP by 1.5x in QoI accuracy	4
II	Bayesian Inversion	Systems with 10K parameters	10
II	Methods for model-form uncertainty	Physics-based methods that outperform GP by 2x in QoI accuracy	12
II	Bayesian Inversion	Systems with 100K parameters	22
II	Methods for model-form uncertainty	Physics-based methods that outperform GP by 5x in QoI accuracy	32
III	Methods for rare events	Prediction accuracy >2x over SOA	8
III	Approximation methods for risk based objective functions	Scalable to 1000 design parameters	18
III	Approximation methods for risk based objective functions	Scalable to 1000 design parameters with theoretical accuracy bounds.	22
III	Methods for rare events	Prediction accuracy >5x over SOA	28
III	Approximation methods for risk based objective functions	Scalable to 1000 design parameters with provably <10% error	36